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Quasibound states of the Green's function for weakly quantized systems

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Abstract. We introduce a technique for calculating quasibound states of a weakly quantized system for which the energy spectrum is non-degenerate and unbounded, above and below. Quasibound states are true stationary states continuously connected with the system bound states by the growth of some parameter. The quasibound state description is found to be unique among the many representations possible for such weakly quantized systems; all other accounts involve decaying (non-stationary) states. In the context of electric fields, examination of the quasibound states leads to an improved understanding of electrical breakdown in matter. In particular, we argue that quasibound states cease to exist for electric fields larger than some critical value $\mathcal{E}_B$—identified with the breakdown field—and that their disappearance is accompanied by a dipole moment which diverges at breakdown as $(\mathcal{E}_B - \mathcal{E})^{-1/2}$.

1. Introduction

The behaviour of a particle bound to a potential well and subjected to the force of a uniform field (electric, gravitational, etc) contains the seeds of a number of interesting and important phenomena. Because the potential energy of a *uniform* field is singular at infinity, the application of a uniform electric field, however weak, creates a potential barrier through which particles can tunnel to escape the attraction of the binding force. This tunnel effect is very small for weak fields. Oppenheimer [1], using an approximate method, estimates that hydrogen atoms dissociate by this mechanism at an astonishingly small rate: 1 in 10^{γ} s, where $\gamma = 10^{10}$ in a field of 1 V cm^{-1}! However, the escape probability, being governed by the transparency of the potential barrier, is strongly field dependent. Zener [2] realized this feature could account for the sudden breakdown of solid dielectrics. In a typical case, he showed that the leakage rate increases as much as one hundred-fold when the field intensifies from 1.0×10^6 V cm^{-1} to 1.1×10^6 V cm^{-1}.

In the language of stationary states this 'leakage' results in a continuum of energy levels. Nearly all the wavefunctions are delocalized, representing unbound states. But embedded in this continuum are special levels, called *quasidiscrete*, for which the wavefunctions, known as *quasibound*, are concentrated in the vicinity of the potential well. Systems giving rise to such states are said to be *weakly quantized*. The quasibound states, being part of a continuum, are unstable; the slightest disturbance will cause them to decay to an unbound state via a radiationless transition. From this viewpoint, Zener breakdown can be ascribed to the large-scale onset of radiationless decay with increasing field. But what of the quasibound states themselves? What happens to *them* as the field intensifies? We know these states

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must be continuously connected to the true bound states by the growth of the field term, so that in weak fields they may be studied using perturbation theory. But with increasing field we meet an unforgiving obstacle: invariably, our perturbation series turns out to be merely asymptotic, and not convergent. This asymptotic nature constitutes a fundamental block to our understanding, beyond which we seemingly cannot penetrate. How, then, do we single out for study the quasibound states in arbitrarily strong fields? In section 2, we provide a surprisingly simple answer to this question for weakly quantized systems in one space dimension. Some consequences, especially for electrical breakdown, are explored, first for a specific model in section 3, and then in a more general context in section 4. In section 5, we summarize the key results and speculate on possible avenues for future work.

2. Quasidiscrete structure and the associated Green's function

In this section we recast Schrödinger's equation for a weakly quantized system as an integral equation. The division between the homogeneous and inhomogeneous versions of this equation will lead us to a description of the quasibound states well beyond the perturbation regime. Results will be given in the context of a uniform electric field, though the method itself transcends any specific application and will be presented so as to emphasize this generality.

The problem may be posed quite generally as follows: we wish to find states of the quasibound variety which satisfy the single-particle Schrödinger equation

$$(\mathcal{H}_0 + V)|\Psi_{\mathrm{E}}\rangle = E|\Psi_{\mathrm{E}}\rangle \tag{1}$$

$\mathcal{H}_0$ includes the kinetic energy, along with the field term giving rise to weak quantization. Accordingly, we take the spectrum of $\mathcal{H}_0$ to be continuous and non-degenerate. V is the binding potential, presumed strong enough to support one or more bound states, and compact, so that the spectrum of $\mathcal{H} = \mathcal{H}_0 + V$ is also continuous and non-degenerate. For a charge q in a uniform electric field $\mathcal{E}$, $\mathcal{H}_0 = p^2/2m - q\mathcal{E}x$, and $V(x)$ can be any potential which vanishes at infinity. Another important example arises in studying vibrations about a point of stable equilibrium. The first term beyond the harmonic approximation is cubic in the displacement. To describe this *anisotropic* oscillator we take $\mathcal{H}_0 = p^2/2m + Cx^3$ and $V(x) = m\omega^2x^2/2$.

We now denote by $|E\rangle$ the eigenstates of $\mathcal{H}_0$. These may be taken orthonormal, $\langle E'|E\rangle = \delta(E' - E)$, and constitute a complete set of states. From them we construct Fourier-transformed states as

$$|\tau\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}E\, \mathrm{e}^{-\mathrm{i}E\tau}|E\rangle. \tag{2}$$

These are also orthonormal $\langle\tau'|\tau\rangle = \delta(\tau' - \tau)$, and form a new basis with the property

$$\mathcal{H}_0|\tau\rangle = \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\tau}|\tau\rangle. \tag{3}$$

Projecting equation (1) onto this basis gives an integro-differential equation for the τ-space wavefunction $\Psi_{\mathrm{E}}(\tau) = \langle\tau|\Psi_{\mathrm{E}}\rangle$:

$$\left(E + \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\tau}\right)\Psi_{\mathrm{E}}(\tau) = \int_{-\infty}^{\infty} \mathrm{d}\tau'\langle\tau|V|\tau'\rangle\Psi_{\mathrm{E}}(\tau').$$

With the help of the integrating factor $\exp(-\mathrm{i}E\tau)$, we can integrate this result over the interval (τ_0, τ) to obtain

$$\Psi_{\mathrm{E}}(\tau) = \mathrm{e}^{\mathrm{i}\mathrm{E}(\tau-\tau_0)}\Psi_{\mathrm{E}}(\tau_0) + \int_{-\infty}^{\infty} \mathrm{d}\tau'\, \Psi_{\mathrm{E}}(\tau')\left[\frac{1}{\mathrm{i}}\int_{\tau_0}^{\tau} \mathrm{d}\tau''\mathrm{e}^{\mathrm{i}\mathrm{E}(\tau-\tau'')}\langle\tau''|V|\tau'\rangle\right]. \tag{4}$$

Equation (4) can be cast in a more familiar form by introducing a Green's function $G_E(\tau, \tau''; \tau_0)$ according to the rules

$$\begin{aligned} G_E(\tau, \tau''; \tau_0) &= -\mathrm{i}\mathrm{e}^{\mathrm{i}E(\tau-\tau'')} \qquad \tau_0 \leqslant \tau'' \leqslant \tau \\ &= +\mathrm{i}\mathrm{e}^{\mathrm{i}E(\tau-\tau'')} \qquad \tau \leqslant \tau'' \leqslant \tau_0 \\ &= 0 \qquad \text{otherwise}. \end{aligned} \tag{5}$$

We now use $G_E(\tau, \tau''; \tau_0)$ to define matrix elements of an operator $G_E(\tau_0)$ as $G_E(\tau, \tau''; \tau_0) = \langle \tau | G_E(\tau_0) | \tau'' \rangle$. Then the bracketed expression in equation (4) becomes $\langle \tau | G_E(\tau_0) V | \tau' \rangle$ and the integral on the right reduces to $\langle \tau | G_E(\tau_0) V | \Psi_E \rangle$. Finally, noting that $\exp(\mathrm{i}E\tau) = (2\pi)^{1/2} \langle \tau | E \rangle$, we recover the Hilbert space version of equation (4):

$$|\Psi_E\rangle = |E\rangle(\sqrt{2\pi}\,\mathrm{e}^{-\mathrm{i}E\tau_0}\Psi_E(\tau_0)) + G_E(\tau_0) V |\Psi_E\rangle. \tag{6}$$

Equation (6) is the desired integral equation formulation of the original Schrödinger equation. The non-uniqueness of the procedure is reflected in the parameter τ_0, which may be any real number. Also, the derivation suggests (correctly) that $\Psi_E(\tau_0)$ is indeterminate; indeed, $\Psi_E(\tau_0)$ reflects a choice of normalization which leads naturally to a division of states into two distinct categories. For *type 1* states, $\Psi_E(\tau_0) \neq 0$ and the bracketed factor in equation (6) can be absorbed into the definition of $|\Psi_E\rangle$ to give the inhomogeneous equation

$$|\Psi_E\rangle = |E\rangle + G_E(\tau_0) V |\Psi_E\rangle. \tag{7}$$

Type 2 states are characterized by $\Psi_E(\tau_0) = 0$, and satisfy the homogeneous equation

$$|\Psi_E\rangle = G_E(\tau_0) V |\Psi_E\rangle. \tag{8}$$

This decomposition depends on the value adopted for τ_0 through the Green's operator $G_E(\tau_0)$ but for every τ_0 the classification is at once mutually exclusive and complete, i.e. a given state is *either* type 1 or type 2, and *all* states are so classified. We will see that different choices for τ_0 lead to alternative descriptions of what is evidently the same physical system, implying that τ_0 is a representation label: *each value taken by τ_0 defines a distinct representation of the weakly quantized system*. Within a representation, type 1 and type 2 states differ markedly in their physical characteristics. In particular, it is the type 2 states alone that vanish with V; alternatively, these must originate with the binding potential. Accordingly, the quasibound states we seek will be found in the type 2 class.

The argument still leaves open the question of how to fix τ_0. Now all stationary states of $\mathcal{H}$ (or, for that matter $\mathcal{H}_0$) have Schrödinger wavefunctions $\langle x | \Psi_E \rangle$ that are real-valued, apart from an overall phase. It follows that $\langle E | \Psi_E \rangle$ may be taken as real. But the type 2 class condition $\Psi_E(\tau_0) = 0$ requires (cf equation (2))

$$\int_{-\infty}^{\infty} \mathrm{d}E\, \mathrm{e}^{\mathrm{i}E\tau_0} \langle E | \Psi_E \rangle = 0.$$

For $\tau_0 \neq 0$ the left-hand side has real and imaginary parts, and both must vanish. This represents one condition too many, suggesting that no type 2 stationary states exist in this case. However, *the choice $\tau_0 = 0$ does admit stationary states of the type 2 class, and these must be the quasibound states*. To obtain them, we solve the homogeneous equation (8) with the Green's operator $G_E(0)$; equivalently, the quasibound states satisfy the Schrödinger equation (1) subject to the added constraint

$$\int_{-\infty}^{\infty} \mathrm{d}E \langle E | \Psi_E \rangle = 0. \tag{9}$$

We turn now to an investigation of the Green operator $G_E(\tau_0)$. From the definition of $G_E(\tau_0)$, we have the formal representation

$$G_E(\tau_0) = \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} d\tau' |\tau\rangle G_E(\tau, \tau'; \tau_0)\langle\tau'|.$$

Substituting equation (5) for $G_E(\tau, \tau'; \tau_0)$ gives

$$\begin{aligned} G_E(\tau_0) &= i\left[\int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\tau_0} d\tau' - \int_{-\infty}^{\infty} d\tau' \int_{\tau'}^{\infty} d\tau\right] e^{iE(\tau-\tau')}|\tau\rangle\langle\tau'| \\ &= i\int_{-\infty}^{\tau_0} d\tau'\, e^{-iE\tau'} \int_{-\infty}^{\infty} d\tau\, e^{iE\tau}|\tau\rangle\langle\tau'| + G_E(-\infty) \\ &= i\sqrt{2\pi}|E\rangle \int_{-\infty}^{\tau_0} d\tau\, e^{-iE\tau}\langle\tau| + G_E(-\infty). \end{aligned} \tag{10}$$

Here $G_E(-\infty)$ symbolizes the Green's operator in the limit as τ_0 approaches negative infinity:

$$G_E(-\infty) = -i\int_{-\infty}^{\infty} d\tau' \int_{\tau'}^{\infty} d\tau\, e^{iE(\tau-\tau')}|\tau\rangle\langle\tau'|.$$

This can be put in a most illuminating form by appealing to equation (3) and invoking the closure property of the basis to obtain

$$\begin{aligned} G_E(-\infty) &= -i\int_0^{\infty} d\tau e^{iE\tau} \int_{-\infty}^{\infty} d\tau'\, |\tau+\tau'\rangle\langle\tau'| \\ &= -i\int_0^{\infty} d\tau\, e^{iE\tau} e^{-i\mathcal{H}_0\tau} \int_{-\infty}^{\infty} d\tau' |\tau'\rangle\langle\tau'| \\ &= -i\int_0^{\infty} d\tau\, e^{iE\tau} e^{-i\mathcal{H}_0\tau}. \end{aligned} \tag{11}$$

We see that $G_E(-\infty)$ is just the Laplace transform of the 'bare' propagator $\exp(-i\mathcal{H}_0\tau)$, and thus is especially suited to describing the evolution of quantum states in cases when the field term is switched on abruptly. For uniform electric fields, this is the Green's operator studied previously by Lukes and Somaratna [3], and Moyer [4]; it leads to type 2 states with complex energies E, and a decaying state picture of the weakly quantized system.

To recover quasibound states, we require the Green's operator that results from taking $\tau_0 = 0$:

$$G_E(0) = i\sqrt{2\pi}|E\rangle \int_{-\infty}^{0} d\tau e^{-iE\tau}\langle\tau| + G_E(-\infty).$$

The coordinate space matrix elements $G_E(x, x'; 0) = \langle x|G_E(0)|x'\rangle$ are calculated from

$$G_E(x, x'; 0) - G_E(x, x'; -\infty) = i\sqrt{2\pi}\langle x|E\rangle \int_{-\infty}^{0} d\tau e^{-iE\tau}\langle\tau|x'\rangle.$$

In the context of uniform fields, $G_E(x, x'; 0)$ can be given in closed form. For a uniform electric field $\mathcal{E}$ the stationary states $\langle x|E\rangle$ are the Airy functions Ai [5]: up to an overall phase, we have

$$\langle x|E\rangle = \frac{\alpha}{\sqrt{q\mathcal{E}}} \mathrm{Ai}(-z) \tag{12}$$

with $z = \alpha(x + E/q\mathcal{E})$ and $\alpha = (2mq\mathcal{E}/\hbar^2)^{1/3}$. Further, from the integral representation of Ai [6] and the inverse of equation (2), we infer

$$\langle x|\tau\rangle = \sqrt{\frac{q\mathcal{E}}{2\pi}}\exp\left(\mathrm{i}q\mathcal{E}x\tau - \mathrm{i}\frac{\hbar^2}{6m}(q\mathcal{E})^2\tau^3\right). \tag{13}$$

Using equations (12) and (13), it is a straightforward matter to show that

$$G_{\mathrm{E}}(x,x';0) - G_{\mathrm{E}}(x,x';-\infty) = \frac{\alpha^2}{|q\mathcal{E}|}\mathrm{Ai}(-z)[\mathrm{i}\pi\,\mathrm{Ai}(-z') - E_0(z')] \tag{14}$$

where $z' = z(x')$. E_0 is a generalized Airy function [7]†; it is real-valued and bounded for all real values of its argument. When equation (14) is added to the closed form for the Green's function $G_{\mathrm{E}}(x,x';-\infty)$ given in [4], we obtain $G_{\mathrm{E}}(x,x';0)$:

$$\begin{aligned} G_{\mathrm{E}}(x,x';0) &= -\frac{\alpha^2}{|q\mathcal{E}|}e_0(z')\mathrm{Ai}(-z) \qquad z \leqslant z' \\ &= -\frac{\alpha^2}{|q\mathcal{E}|}[E_0(z')\mathrm{Ai}(-z) + \pi\,\mathrm{Ai}(-z')\mathrm{Bi}(-z)] \qquad z \geqslant z'. \end{aligned} \tag{15}$$

Bi is the Airy function companion to Ai (the second independent solution to Airy's equation), and $e_0(z) = E_0(z) + \pi\,\mathrm{Bi}(-z)$ is yet another generalized Airy function. The Green's function of equation (15) was first proposed by us in 1970, following a somewhat obscure and less inclusive approach [8].

It is no accident that $G_{\mathrm{E}}(x,x';0)$ is a real-valued function, as can be seen by writing the homogeneous equation (8) in the coordinate basis (now with $\tau_0 = 0$):

$$\Psi_{\mathrm{E}}(x) = \int_{-\infty}^{\infty}\mathrm{d}x'\,G_{\mathrm{E}}(x,x';0)V(x')\Psi_{\mathrm{E}}(x'). \tag{16}$$

With $G_{\mathrm{E}}(x,x';0)$ real, equation (16) admits stationary-state (quasibound) wavefunctions $\Psi_{\mathrm{E}}(x)$ with real (quasidiscrete) energies E. Furthermore, no choice other than $\tau_0 = 0$ leads to a Green's function with this property. Suppose in contrast that $\tau_1 \neq 0$ also resulted in a real-valued Green's function $G_{\mathrm{E}}(x,x';\tau_1)$. Then, from equation (10), the difference

$$G_{\mathrm{E}}(x,x';\tau_1) - G_{\mathrm{E}}(x,x';0) = \mathrm{i}\sqrt{2\pi}\langle x|E\rangle\int_0^{\tau_1}\mathrm{d}\tau\,\mathrm{e}^{-\mathrm{i}E\tau}\langle\tau|x'\rangle \tag{17}$$

would have to be real for all values of x and x'. But equations (12) and (13) indicate that the right-hand side of equation (17) has an imaginary part proportional to

$$\int_0^{\tau_1}\mathrm{d}\tau\cos\left[(q\mathcal{E}x' + E)\tau - \frac{\hbar^2}{6m}(q\mathcal{E})^2\tau^3\right]. \tag{18}$$

For all $\tau_1 \neq 0$, this integral defines an analytic function of x' (having only isolated zeros); thus, the supposition that both $G_{\mathrm{E}}(x,x';\tau_1)$ and $G_{\mathrm{E}}(x,x';0)$ are everywhere real must be false. We conclude that *the Green's function of equation (15), when used with equation (16) affords a description of the quasibound states in uniform fields of any strength.*

One final remark concerning uniqueness is in order. We know that any Green operator G_{E} for $\mathcal{H}_0$ must satisfy

$$(E - \mathcal{H}_0)G_{\mathrm{E}} = 1 \tag{19}$$

for equations (7) and/or (8) to be valid. Assuming a solution G_{E} can be found which meets the usual boundedness and continuity conditions, it is often not unique. Another

† These are related to the functions Gi, Hi introduced in [6] by the formulas $E_0(z) = -\pi\,\mathrm{Gi}(-z)$; $e_0(z) = \pi\,\mathrm{Hi}(-z)$.

Green's operator with the same properties can be constructed as $G_E + |E\rangle\langle\Gamma|$, where $|E\rangle$ is an eigenstate of $\mathcal{H}_0$ and $\langle\Gamma|$ is an *arbitrary* state. For true bound states (having discrete energies) this poses no problem because we are interested in G_E at the perturbed energies only, and E would almost never be an eigenvalue of both $\mathcal{H}_0$ *and* $\mathcal{H} = \mathcal{H}_0 + V$. The same cannot be said for the quasibound states of weakly quantized systems, where even requiring real-valued matrix elements $\langle x|G_E|x'\rangle$ clearly does not limit the choice to a single G_E. This uniqueness problem, as reflected in the state $\langle\Gamma|$, is compounded by the observation that—at least for uniform fields—the unperturbed eigenstate $|E\rangle$ is asymptotically small to *all orders* in the field parameter! Thus, further requiring G_E to reproduce the results of perturbation theory to *any* order still does nothing to mitigate the non-uniqueness inherent in this approach.

By comparison, equation (10) effectively limits $\langle\Gamma|$ to

$$\langle\Gamma| = \mathrm{i}\sqrt{2\pi}\int_{-\infty}^{\tau_0} \mathrm{d}\tau\, \mathrm{e}^{-\mathrm{i}E\tau}\langle\tau|. \tag{20}$$

The limitation imposed by equation (20) has subtle origins going back to equation (6), where it appears as the bracketed term so essential for enforcing the type 1–type 2 state classification that distinguishes the quasibound states from the pack. The suggestion is simply this: *there are a restricted number of ways to represent a weakly quantized system that rigorously preserve the identity of quasibound states as the system parameters are varied*. These ways are indexed here by the (continuous) label τ_0; equivalently, we may say that each value of τ_0 generates a proper representation of the weakly quantized system. But again, only $\tau_0 = 0$ results in true quasibound states, i.e. stationary states having real energies.

The expected connectivity of the quasibound states defined by equation (16) to the bound states of $V(x)$ is verified for the example of section 3; further, the behaviour in strong fields of the quasibound state found there will lead us to an unambiguous definition of electrical breakdown at the microscopic level.

3. Quasibound state of the delta function well

The understanding of new concepts traditionally begins with the study of idealized approximations to reality which, though crude, yield to the exact methods of analysis. In this spirit, we turn now to an investigation of the quasibound state for the simplest non-trivial potential—a delta function well.

The delta well is described by the potential function $V(x) = -S\delta(x)$, with $S > 0$ a parameter measuring the strength of the well. In the absence of an electric field, there is just one bound state with energy $E_0 = -mS^2/2\hbar^2$. For $\mathcal{E} > 0$, the quasibound state is given by equation (16) which, in this case, reduces to the algebraic equation

$$\Psi_E(x) = -SG_E(x, 0; 0)\Psi_E(0).$$

Solutions exist only for those energies E satisfying $1 = -SG_E(0, 0; 0)$ or, using the expression (15) for $G_E(x, x'; 0)$,

$$1 = S\frac{\alpha^2}{|q\mathcal{E}|}e_0(z_0)\mathrm{Ai}(-z_0). \tag{21}$$

Here $z_0 = z|_{x=0} = \alpha E/q\mathcal{E}$. Even in this simple example, we must resort to graphical or numerical techniques to obtain the quasidiscrete energies. There are, however, two limiting cases which can be handled analytically.

The first is the realm of weak fields. As $\mathcal{E} \to 0$, $E \to E_0(< 0)$ and $z_0 \to -\infty$. Thus, we may employ the asymptotic expansions for $\mathrm{Ai}(-z)$ and $e_0(z) \sim \pi \mathrm{Bi}(-z)$ to obtain [6]

$$e_0(z)\mathrm{Ai}(-z) \sim \frac{1}{2\sqrt{z}}\left(1 + \frac{5}{32}\frac{1}{z^3}\right) + \mathrm{O}\left(\frac{1}{z^5}\right).$$

With some manipulation, equation (21) can be brought to the more transparent form

$$\sqrt{\frac{E}{E_0}} = 1 - \frac{5}{32}\frac{\hbar^2}{2m}\frac{(q\mathcal{E})^2}{E^3} + \mathrm{O}(\mathcal{E}^4)$$

from which the zeroth approximation $E \approx E_0$ readily emerges. Substituting this back into the right-hand side of the equation yields the next order approximant

$$E \approx E_0 - \frac{5}{16}\frac{\hbar^2}{2mE_0^2}(q\mathcal{E})^2. \tag{22}$$

In equation (22) we recover the result of Rayleigh–Schrödinger perturbation theory carried to second order in $\mathcal{E}$. (No linear term arises due to the reflection symmetry of the potential.) The development is clearly asymptotic in the electric field strength.

We can also obtain strong field results by observing that $f(z_0) = e_0(z_0)\mathrm{Ai}(-z_0)$ is bounded for all z_0. Thus, the equality in equation (21) can be maintained only if the field strength is less than some critical value $\mathcal{E}_\mathrm{B}$. For $\mathcal{E} > \mathcal{E}_\mathrm{B}$ no solution exists; the electric field has destroyed the quasibound state. Moreover, the argument implies that destruction obtains for that value of z_0 which makes $f(z_0)$ a maximum, and this occurs for $z_0 = 0$. Noting that

$$f(0) = e_0(0)\mathrm{Ai}(0) = \frac{2\pi}{9}\frac{3^{1/6}}{\Gamma^2(2/3)} = 0.457\,240\,39\ldots \tag{23}$$

we find from equation (22) and (23) the critical field $\mathcal{E}_\mathrm{B}$:

$$|q\mathcal{E}_\mathrm{B}| = \left(\frac{2\pi}{9}\right)^3 \frac{3^{1/2}}{\Gamma^6(2/3)}\left(\frac{2m}{\hbar^2}\right)^2 S^3. \tag{24}$$

Since $z_0 = 0$ here, we see also that $E(\mathcal{E}_\mathrm{B}) = 0$. This value for $E(\mathcal{E}_\mathrm{B})$ is reasonable, since then the bound charge has surely acquired sufficient energy to escape the 'pull' of its confining well.

For general computation, it is advantageous to rewrite equation (21) in parametric form, using z_0 as the parameter:

$$\begin{aligned} \frac{E}{|E_0|} &= 4z_0 f^2(z_0) \\ \frac{\mathcal{E}}{\mathcal{E}_\mathrm{B}} &= \frac{f^3(z_0)}{f^3(0)}. \end{aligned} \tag{25}$$

These last equations are very convenient to use. For each value of z_0 we find E from the first of equations (25) and $\mathcal{E}$ from the second. The full curve $E(\mathcal{E})$ is generated by allowing z_0 to range from minus infinity to zero. Indeed, for the delta function well, the entire effect of the electric field on the quasidiscrete levels can be neatly summarized in one graph (figure 1), with E_0 and $\mathcal{E}_\mathrm{B}$ serving merely to fix the scales appropriately. The asymptotic formula equation (22), which can be expressed as

$$\frac{E}{|E_0|} = -1 - 20 f^6(0)\left(\frac{\mathcal{E}}{\mathcal{E}_\mathrm{B}}\right)^2$$

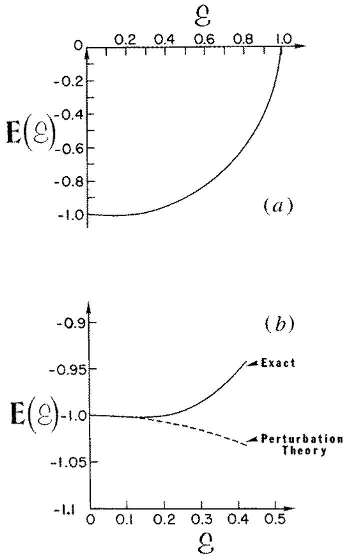

Figure 1. The quasidiscrete energy $E(\mathcal{E})$ for the delta function well, in units of the binding energy $|E_0|$. The electric field strength $\mathcal{E}$ is recorded in units of the breakdown field $\mathcal{E}_B$. (*a*) Full curve, showing level termination at $\mathcal{E} = \mathcal{E}_B$. (*b*) The weak field regime, showing the comparison with the result of perturbation theory carried to second order in $\mathcal{E}$.

is shown in figure 1(*b*) for comparison. Even on this expanded scale, the two curves are nearly indistinguishable for $\mathcal{E} \lesssim 0.15\,\mathcal{E}_B$; beyond this the true curve turns rapidly upward and terminates at $\mathcal{E} = \mathcal{E}_B$, in agreement with our earlier remarks. In practical applications, the perturbation result fares badly only above electric fields $\mathcal{E} \sim 10^7$ V cm^{-1}.

Nevertheless, the strong field regime is one of genuine theoretical interest, encompassing as it does the destruction of the quasibound state. Consider the behaviour of the induced dipole moment P, which arises because the electric field distorts the (initially symmetric) charge 'cloud'. For our delta function model we must calculate

$$P = \langle qx \rangle = \frac{\langle \Psi_E | qx | \Psi_E \rangle}{\langle \Psi_E | \Psi_E \rangle} \tag{26}$$

for the quasibound state $|\Psi_E\rangle$. In coordinate space equation (26) becomes a ratio of two divergent integrals since the quasibound state, being embedded in a continuum, is not square-integrable. Fortunately, we may avoid these unpleasantries by appealing to the Hellmann–Feynman Theorem [9], which allows us to write

$$P(\mathcal{E}) = -\frac{\partial E}{\partial \mathcal{E}} \tag{27}$$

with $E(\mathcal{E})$ the energy of the quasibound state. Equation (27) makes the study of the dipole moment an easy task. For weak fields, equation (22) shows that $P(\mathcal{E})$ depends linearly on $\mathcal{E}$; the coefficient of proportionality

$$\frac{5}{16}\frac{q^2\hbar^2}{mE_0^2}$$

is the polarizability of the delta well.

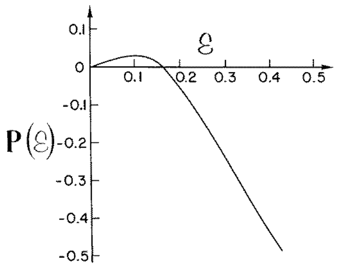

Figure 2. The induced dipole moment $P(\mathcal{E})$ for the delta function well. Polarization reversal occurs for $\mathcal{E} = 0.15\mathcal{E}_B$, where $P(\mathcal{E})$ becomes zero. $P(\mathcal{E})$ diverges for $\mathcal{E} = \mathcal{E}_B$ (not shown).

In stronger fields $P(\mathcal{E})$, like $E(\mathcal{E})$, must be determined numerically. Using equations (25), we obtain

$$P = -\frac{\partial E/\partial z_0}{\partial \mathcal{E}/\partial z_0} = -\frac{4|E_0|f^3(0)}{3\mathcal{E}_B}\left(\frac{2z_0}{f(z_0)} + \frac{1}{f'(z_0)}\right). \tag{28}$$

Here as before, $f(z_0) = e_0(z_0)\mathrm{Ai}(-z_0)$ and prime ($'$) denotes differentiation with respect to the argument. Again, z_0 parametrizes the functional dependence $P(\mathcal{E})$, with $\mathcal{E}$ still given by the second of equations (25). The resulting curve, with an appropriate scale adjustment, is figure 2.

$P(\mathcal{E})$ diverges at $\mathcal{E}_B$, since $z_0 = 0$ is a point of zero slope for $f(z_0)$. Thus, at $\mathcal{E}_B$ the average position $\langle x \rangle$ becomes infinite; the system has been literally torn apart by the electric field! The implication is inescapable: for $\mathcal{E} = \mathcal{E}_B$, *electrical breakdown has occurred, and* $\mathcal{E}_B$ *should be identified with the breakdown field.* In the neighbourhood of $\mathcal{E}_B$, z_0 is small and we can approximate

$$P \approx -\frac{4|E_0|f^3(0)}{3\mathcal{E}_B f''(0)}\frac{1}{z_0}$$

$$\frac{\mathcal{E} - \mathcal{E}_B}{\mathcal{E}_B} \approx \frac{3f''(0)}{2f(0)}z_0^2.$$

Eliminating z_0 from this pair shows that $P(\mathcal{E})$ diverges at $\mathcal{E}_B$ like $(\mathcal{E}_B - \mathcal{E})^{-1/2}$. Moreover, since $f''(0)$ is negative ($z_0 = 0$ is a maximum for $f(z_0)$), $P(\mathcal{E})$ is *less than zero* in these strong fields; the system undergoes a *polarization reversal* prior to electrical breakdown! Polarization reversal is likely to be an artifact introduced by the delta function singularity; indeed, it is easy to see why the delta function model must exhibit such a peculiarity. We have already argued that the value zero for the energy $E(\mathcal{E}_B)$ at breakdown is reasonable. Add to this the observation that the quasidiscrete level is initially depressed (as shown by perturbation theory) and the conclusion is inescapable: the curve $E(\mathcal{E})$ must pass through a minimum. Thus, $P(\mathcal{E}) = -\partial E/\partial \mathcal{E}$ returns to zero and thereafter changes sign.

Finally, we show as figure 3 the quasibound wavefunctions at several important field values. For a fixed electric field, all well configurations are incorporated into a single graph by plotting $\Psi_E(x)$ versus the dimensionless variable κx, where κ is the decay length of the unperturbed bound state ($\kappa^2 = 2m|E_0|/\hbar^2$). The wavefunctions, normalized as $\Psi_E(0) = 1$, can be written

$$\Psi_E(x) = \frac{\mathrm{Ai}(-z)}{\mathrm{Ai}(-z_0)} \qquad x \leqslant 0$$

$$= \frac{E_0(z_0)}{f(z_0)}\mathrm{Ai}(-z) + \frac{\pi}{e_0(z_0)}\mathrm{Bi}(-z) \qquad x \geqslant 0 \tag{29}$$

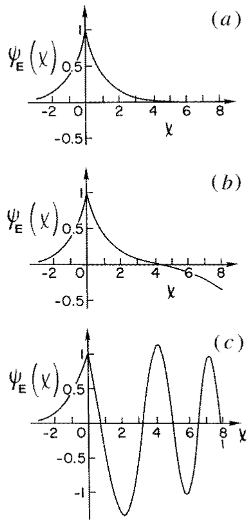

Figure 3. The quasibound state wavefunction $\psi_{\rm E}(x)$ of the delta well for selected electric field values. (*a*) For $\mathcal{E} \approx \mathcal{E}_{\rm B}/50$ the wavefunction is indistinguishable from the unperturbed bound state. (*b*) The wavefunction just prior to polarization reversal, $\mathcal{E} = 0.15\mathcal{E}_{\rm B}$. (*c*) The wavefunction at $\mathcal{E} = \mathcal{E}_{\rm B}$, where complete electrical breakdown is attained.

with $z = z_0 + 2f(z_0)\kappa x$. Figure 3(*a*) shows the wavefunction for $\mathcal{E} \approx \mathcal{E}_{\rm B}/50$; in these weak fields it is indistinguishable from the unperturbed bound state $\Psi_{\rm E}(x) = \exp(-\kappa|x|)$. The wavefunction just prior to polarization reversal is illustrated in figure 3(*b*). At this point, some delocalization is noticeable, although features of the bound state still predominate. In contrast, no trace of a localized state remains in figure 3(*c*), where complete electrical breakdown has been attained.

4. Singular behaviour of the dipole moment near breakdown

For the delta well of section 3, we found a quasibound state continuously connected with the lone bound state whose disappearance at the critical field $\mathcal{E}_{\rm B}$ was accompanied by a dipole moment $P(\mathcal{E})$ diverging at $\mathcal{E}_{\rm B}$ like $(\mathcal{E}_{\rm B} - \mathcal{E})^{-1/2}$. In this section we show that this singular behaviour of $P(\mathcal{E})$ near $\mathcal{E}_{\rm B}$ is universal, independent of the details of the interaction potential $V(x)$.

The argument proceeds by using the relation $E_0(z) = e_0(z) - \pi \mathrm{Bi}(-z)$ to rewrite equation (16) as a Volterra integral equation

$$\Psi(z) = C\frac{\alpha}{q\mathcal{E}}\mathrm{Ai}(-z) + \frac{\alpha}{q\mathcal{E}}\int_{-\infty}^{z} \mathrm{d}z'\,K(z,z')\Psi(z')$$

where $\Psi(z) \equiv \Psi_{\rm E}(x(z))$. The kernel $K(z,z')$ and constant C are given by

$$K(z,z') = \pi[\mathrm{Ai}(-z)\mathrm{Bi}(-z') - \mathrm{Bi}(-z)\mathrm{Ai}(-z')]V_{\rm E}(z')$$

$$C = -\int_{-\infty}^{\infty} \mathrm{d}z\, e_0(z)V_{\rm E}(z)\Psi(z)$$

with $V_{\rm E}(z) \equiv V(x(z))$. Iteration generates the formal solution $\Psi(z) = C\phi(z)$ where

$$\phi(z) = \sum_{n=0}^{\infty}\left(\frac{\alpha}{q\mathcal{E}}\right)^{n+1}\phi_n(z)$$

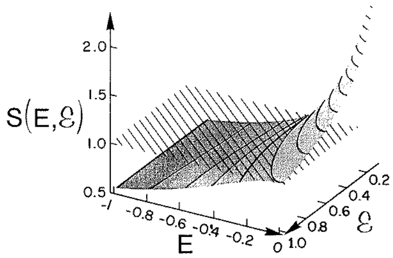

Figure 4. Sketch of the 'eigensurface' $S(E,\mathcal{E})$ (shaded region) for a general potential energy $V(x)$. The quasidiscrete energies $E(\mathcal{E})$ are given by the intersection of this surface with the plane at $S=1$. The 'smoothness' of $S(E,\mathcal{E})$ implies that level termination is accompanied by a divergent dipole moment.

$$\phi_n(z)=\int_{-\infty}^{z}\mathrm{d}z'K(z,z')\phi_{n-1}(z')\qquad \phi_0(z)=\mathrm{Ai}(-z). \tag{30}$$

The equation for the quasidiscrete energies follows from the definition of C:

$$1=-\int_{-\infty}^{\infty}\mathrm{d}z\,e_0(z)V_{\mathrm{E}}(z)\phi(z). \tag{31}$$

It is enlightening to regard the preceding equation as the intersection of the 'eigensurface'

$$S(E,\mathcal{E})=-\int_{-\infty}^{\infty}\mathrm{d}z\,e_0(z)V_{\mathrm{E}}(z)\phi(z) \tag{32}$$

with the plane $S=1$. In the discussion to follow, we assume $S(E,\mathcal{E})$ is 'smooth' in the region of interest, i.e. that $S(E,\mathcal{E})$ and its first derivatives are continuous. The validity of this assumption, as well as the manipulations leading to equation (30) are justified if $V(x)$ is continuous and $\mathrm{d}V/\mathrm{d}x$ vanishes at infinity faster than $|x|^{-3/2}$. With the same restrictions, it can be shown that $S(E,\mathcal{E})$ becomes arbitrarily small for $\mathcal{E}$ sufficiently large, thereby guaranteeing through equation (31) that each quasidiscrete level must terminate at some field value. These demands on $V(x)$ are surely excessive, as the example of section 3 indicates; nonetheless they do admit a broad and important class of potentials.

The 'smoothness' of $S(E,\mathcal{E})$ furnishes a direct link between the destruction of a quasibound state (via level termination) and the divergence of its dipole moment. To see this, we must interpret the termination of a quasidiscrete level in terms of the topological properties of the eigensurface. This can be done by visualizing the intersection of $S(E,\mathcal{E})$ with a plane of constant $\mathcal{E}$ as this plane advances in the direction of increasing field (figure 4). As $\mathcal{E}$ grows, the curve of intersection varies, but the smoothness of the eigensurface implies that, for the critical field $\mathcal{E}_{\mathrm{B}}$, the curve $S(E,\mathcal{E}_{\mathrm{B}})$ possesses a maximum or minimum at the corresponding ionization energy $E_{\mathrm{B}}=E(\mathcal{E}_{\mathrm{B}})$:

$$\frac{\partial S}{\partial E}=0\qquad \frac{\partial^2 S}{\partial E^2}\neq 0\qquad \text{at } (E_{\mathrm{B}},\mathcal{E}_{\mathrm{B}}). \tag{33}$$

Furthermore, we can assume

$$\frac{\partial S}{\partial \mathcal{E}}\neq 0\qquad \text{at } (E_{\mathrm{B}},\mathcal{E}_{\mathrm{B}}) \tag{34}$$

for if this were not so, the surface $S(E,\mathcal{E})$ would exhibit a local peak, valley, or saddle point at $(E_{\mathrm{B}},\mathcal{E}_{\mathrm{B}})$. A peak or valley implies level termination with a *decrease* as well as an increase in $\mathcal{E}$, and so may be excluded. A saddle point describes *level crossing*, and is forbidden by the assumed non-degeneracy of the energy spectrum. Also, we note that the signs of $\partial^2 S/\partial E^2$ and $\partial S/\partial \mathcal{E}$, when evaluated at $(E_B, \mathcal{E}_B)$, are correlated: if $S(E, \mathcal{E}_B)$ has a maximum (minimum) at $E = E_B$, then $\partial S/\partial \mathcal{E}$ evaluated at $(E_B, \mathcal{E}_B)$ must be negative (positive) for level termination to occur. It follows that $\partial^2 S/\partial E^2$ and $\partial S/\partial \mathcal{E}$ are either both positive or both negative, and that their ratio is always positive.

The divergence of the dipole moment at breakdown is now readily demonstrated. In the solution plane $S(E, \mathcal{E}) = 1$, we have $\mathrm{d}S = \partial S/\partial E \,\mathrm{d}E + \partial S/\partial \mathcal{E} \,\mathrm{d}\mathcal{E} = 0$. Thus,

$$P = -\frac{\partial E}{\partial \mathcal{E}} = \frac{\partial S}{\partial \mathcal{E}} \bigg/ \frac{\partial S}{\partial E}$$

and by conditions (33) and (34), P diverges at the critical point $(E_B, \mathcal{E}_B)$. The form of the divergence follows directly from a Taylor expansion of $S(E, \mathcal{E})$ around $(E_B, \mathcal{E}_B)$.

Remembering that $S(E_B, \mathcal{E}_B) = 1$, we find

$$E(\mathcal{E}) = E_B \pm \beta(\mathcal{E}_B - \mathcal{E})^{1/2} + \mathrm{O}(\mathcal{E}_B - \mathcal{E}) \tag{35}$$

where

$$\beta^2 = 2\frac{\partial S}{\partial \mathcal{E}} \bigg/ \frac{\partial^2 S}{\partial E^2} \qquad \text{evaluated at } (E_B, \mathcal{E}_B) \tag{36}$$

is a positive number by our previous remarks. Thus, near the critical field $\mathcal{E}_B$, the dipole moment $P(\mathcal{E}) = -\partial E/\partial \mathcal{E}$ diverges as

$$P(\mathcal{E}) = \pm\frac{\beta}{2}(\mathcal{E}_B - \mathcal{E})^{-1/2} + \mathrm{O}(1). \tag{37}$$

Let us pause for a moment to reflect upon this result. Statements (33)–(37) are just a clumsy analytical way of saying what is geometrically obvious: given that the solution curve $E(\mathcal{E})$ originates from the intersection of a plane with a smooth surface, then any solution which terminates must do so with infinite slope (cf figure 4). The type of singularity reflects the dimensionality of the surface—in this case two. Thus, level termination and the dimensionality of the eigensurface alone dictate the prediction of equation (37).

5. Conclusion

We have presented a technique for calculating quasibound states of a weakly quantized system for which the energy spectrum is non-degenerate and unbounded, above and below. Besides satisfying Schrödinger's equation, the quasibound states are subject to the added constraint imposed by equation (9), namely

$$\int_{-\infty}^{\infty} \mathrm{d}E \langle E|\psi_E\rangle = 0.$$

Equivalently, quasibound states may be sought as solutions to a homogeneous integral equation, using the Green's operator of equation (10) in the special case $\tau_0 = 0$. More generally, τ_0 labels representations; all non-zero choices for τ_0 result in alternative descriptions of the weakly quantized system in terms of localized states that are not truly stationary, but decay over time. The conventional treatment corresponds to the case $\tau_0 = -\infty$.

In the context of electric fields, examination of the quasibound states leads to an improved understanding of electrical breakdown in matter. From the example of a charge bound by a delta function well and subject to a uniform electric field, we are able to arrive at the following generalizations:

• quasibound states cease to exist for electric fields larger than some critical value $\mathcal{E}_B$, identified with the breakdown field for the system.

• The associated quasidiscrete energy level terminates at the value of the breakdown field.

• Termination of a quasidiscrete level is invariably accompanied by a dipole moment which diverges at breakdown as $(\mathcal{E}_B - \mathcal{E})^{-1/2}$.

Several points still require clarification. How quasibound states may be realized in practice remains an open question. It is tempting to think that the *adiabatic* growth of $\mathcal{E}$ starting from a bound state may result in evolution to the corresponding quasibound state, but at present this is only conjecture. Other, more straightforward, extensions of the present work are also indicated. These include the treatment of weakly quantized systems with fundamentally different spectra (e.g. bounded below but not above), as well as the possibility of generalizing the method from one to three space dimensions. Both will be taken up in future publications.

References

[1] Oppenheimer J R 1928 *Phys. Rev.* **31** 80
[2] Zener C 1934 *Proc. R. Soc.* A **145** 529
[3] Lukes T and Somaratna K T S 1969 *J. Phys. C: Solid State Phys.* **2** 586
[4] Moyer C A 1973 *J. Phys. C: Solid State Phys.* **6** 1461
[5] Landau L D and Lifshitz E M 1977 *Quantum Mechanics* 3rd edn (Oxford: Pergamon) section 24
[6] Abramowitz M and Stegun I A 1965 *Handbook of Mathematical Functions* (New York: Dover) pp 446–8
[7] Tumarkin S A 1959 *J. Appl. Math. Mech.* **23** 1556
[8] Moyer C A 1970 *Ann. Phys., NY* **61** 242
[9] Merzbacher E 1970 *Quantum Mechanics* 2nd edn (New York: Wiley) p 442